CHBE 305

COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING

Spring 2013

Instructor

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Office Hours: MW 4:30 - 5:30 PM

Course Contents

1. Introduction. Approximations and round-off errors; truncation errors, Taylor series.
2. Systems of linear algebraic equations: Introduction; Gauss elimination, LU decomposition; inversion of matrices; error analysis and system condition; band matrices; iterative solution; Gauss-Seidel method.
3. Solution of non-linear equations: bisection method; false-position method; simple fixed-point iteration; Newton-Raphson method; secant method; multiple roots; systems on nonlinear equations; roots of polynomials.
4. Curve fitting: Least squares regression; linear regression; polynomial regression; multiple linear regression; general linear least squares; nonlinear regression. Interpolation; spline interpolation.
5. Optimization: One-dimensional unconstrained optimization; golden-section search; quadratic interpolation; Newton's method. Multidimensional unconstrained optimization: direct methods; gradient methods. Constrained optimization: linear programming; nonlinear constrained optimization.
6. Numerical solution of ordinary differential equations: Euler's methods; Runge-Kutta methods; adaptive Runge-Kutta methods; systems of equations; stiffness; multistep methods; general methods for boundary values problems; eigenvalue problems.

Textbook

S. C. Chapra and R.R. Canale, "Numerical methods for Engineers." Sixth Edition, McGraw-Hill (2010).

Recitation Sessions (Computer Labs)

A 2-hour recitation session will be held every week. The class will be divided in sections for the recitations. Attendance of recitations is mandatory.

Computer Programming

Unless otherwise specified, students are free to use either MATLAB or Fortran for the solution of homework problems.

Homework Assignments

Six to eight homework problem sets will be assigned during the semester. Problems will involve both theoretical analysis and computer programing.

Homework Policy

- Late homework will be penalized, unless prior permission has been obtained from the instructor.
- Homework that is more than four days late will not be accepted.
- You can get up to two "free extensions" of homework due dates by notifying the instructor and the TAs in advance of the due date. For each of the free extensions, you may push the due date by no more than two class periods. You cannot use both free extensions for the same homework.
- There will be no "regrades."

Quizzes

There will be two short quizzes to test the students' understanding of key concepts. The quizzes will not require the use of computers and are tentatively set for February 22 and April 19.

Team Project

Students will work in teams to design a set of "computer-based experiments" and analyze the data in order to identify the kinetics of an unknown reaction. This information will then be used to design a chemical reactor system that meets certain specifications. Each team will make a formal presentation of their design and submit a written report by the last day of finals (May 1, 2013).